Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1612bxr

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

```
 NEWS  1          Web Page for STN Seminar Schedule - N. America
 NEWS  2  AUG 06  CAS REGISTRY enhanced with new experimental property tags
 NEWS  3  AUG 06  FSTA enhanced with new thesaurus edition
 NEWS  4  AUG 13  CA/CAplus enhanced with additional kind codes for granted
                  patents
 NEWS  5  AUG 20  CA/CAplus enhanced with CAS indexing in pre-1907 records
 NEWS  6  AUG 27  Full-text patent databases enhanced with predefined
                  patent family display formats from INPADOCDB
 NEWS  7  AUG 27  USPATOLD now available on STN
 NEWS  8  AUG 28  CAS REGISTRY enhanced with additional experimental
                  spectral property data
 NEWS  9  SEP 07  STN AnaVist, Version 2.0, now available with Derwent
                  World Patents Index
 NEWS 10  SEP 13  FORIS renamed to SOFIS
 NEWS 11  SEP 13  INPADOCDB enhanced with monthly SDI frequency
 NEWS 12  SEP 17  CA/CAplus enhanced with printed CA page images from
                  1967-1998
 NEWS 13  SEP 17  CAplus coverage extended to include traditional medicine
                  patents
 NEWS 14  SEP 24  EMBASE, EMBAL, and LEMBASE reloaded with enhancements
 NEWS 15  OCT 02  CA/CAplus enhanced with pre-1907 records from Chemisches
                  Zentralblatt
 NEWS 16  OCT 19  BEILSTEIN updated with new compounds
 NEWS 17  NOV 15  Derwent Indian patent publication number format enhanced
 NEWS 18  NOV 19  WPIX enhanced with XML display format
 NEWS 19  NOV 30  ICSD reloaded with enhancements
 NEWS 20  DEC 04  LINPADOCDB now available on STN
 NEWS 21  DEC 14  BEILSTEIN pricing structure to change
 NEWS 22  DEC 17  USPATOLD added to additional database clusters
 NEWS 23  DEC 17  IMSDRUGCONF removed from database clusters and STN
 NEWS 24  DEC 17  DGENE now includes more than 10 million sequences
 NEWS 25  DEC 17  TOXCENTER enhanced with 2008 MeSH vocabulary in
                  MEDLINE segment
 NEWS 26  DEC 17  MEDLINE and LMEDLINE updated with 2008 MeSH vocabulary
 NEWS 27  DEC 17  CA/CAplus enhanced with new custom IPC display formats
 NEWS 28  DEC 17  STN Viewer enhanced with full-text patent content
                  from USPATOLD
 NEWS 29  JAN 02  STN pricing information for 2008 now available

 NEWS EXPRESS  19 SEPTEMBER 2007:  CURRENT WINDOWS VERSION IS V8.2,
               CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
               AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.

 NEWS HOURS    STN Operating Hours Plus Help Desk Availability
 NEWS LOGIN    Welcome Banner and News Items
```

Updated Search

NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 23:40:03 ON 06 JAN 2008

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 23:40:15 ON 06 JAN 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 4 JAN 2008 HIGHEST RN 960040-46-4
DICTIONARY FILE UPDATES: 4 JAN 2008 HIGHEST RN 960040-46-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=> file casreact

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	5.52	5.73

FILE 'CASREACT' ENTERED AT 23:47:18 ON 06 JAN 2008
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT
COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications.

FILE CONTENT:1840 - 5 Jan 2008 VOL 148 ISS 2

Updated Search

New CAS Information Use Policies, enter HELP USAGETERMS for details.

```
************************************************************
*                                                          *
*     CASREACT now has more than 13.8 million reactions    *
*                                                          *
************************************************************
```

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

```
=>
Uploading C:\Documents and Settings\brobinson1\My Documents\stnweb\Queries\acvg.str

L1      STRUCTURE UPLOADED

=> s l1
SAMPLE SEARCH INITIATED 23:48:06 FILE 'CASREACT'
SCREENING COMPLETE -       60 REACTIONS TO VERIFY FROM        8 DOCUMENTS

100.0% DONE      60 VERIFIED       0 HIT RXNS                      0 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED VERIFICATIONS:       736 TO     1664
PROJECTED ANSWERS:               0 TO        0

L2            0 SEA SSS SAM L1 (     0 REACTIONS)

=> s l1 full
THE ESTIMATED SEARCH COST FOR FILE 'CASREACT' IS 117.50 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 23:48:11 FILE 'CASREACT'
SCREENING COMPLETE -     1127 REACTIONS TO VERIFY FROM      175 DOCUMENTS

100.0% DONE    1127 VERIFIED      43 HIT RXNS                      9 DOCS
SEARCH TIME: 00.00.01

L3            9 SEA SSS FUL L1 (    43 REACTIONS)

=> s l3 and shapiro, r?/au
            50 SHAPIRO, R?/AU
L4           0 L3 AND SHAPIRO, R?/AU

=> d l3, ibib abs fhit, 1-9


L3   ANSWER 1 OF 9  CASREACT  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:         144:212761  CASREACT
TITLE:                    Preparation of (1S,5S)-3-(5,6-dichloro-3-pyridinyl)-
                          3,6-diazabicyclo[3.2.0]heptane as a nicotinic
                          acetylcholine receptor ligand useful as an effective
                          analgesic agent
INVENTOR(S):              Buckley, Michael J.; Ji, Jianguo; Zhang, Geoff G. Z.;
                          Henry, Rodger F.; Wang, Weili W.; Wayne, Gregory S.;
                          Li, Wenke; Towne, Timothy B.; Wittenberger, Steven J.;


Updated Search
```

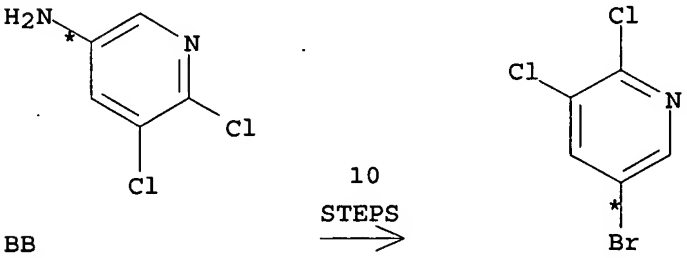
Hannick, Steven M.; Kotecki, Brian J.; Macri, Bryan S.; Robbins, Timothy A.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 45 pp., Cont.-in-part of U.S. Ser. No. 898,441.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2006035936	A1	20060216	US 2005-176087	20050707
US 2004242644	A1	20041202	US 2004-851917	20040521
US 2005261348	A1	20051124	US 2004-898441	20040723
PRIORITY APPLN. INFO.:			US 2004-851917	20040521
			US 2004-898441	20040723
			US 2003-473530P	20030527

AB The present invention discloses (1S,5S)-3-(5,6-dichloro-3-pyridinyl)-3,6-diazabicyclo[3.2.0]heptane (I) and salts thereof, methods for their preparation and their use to treat pain and other disorders associated with the nicotinic acetylcholine receptor. Compared to related analogs, I is a potent analgesic with reduced side effect liability. Compound I was prepared in 10 steps starting from 2-hydroxy-5-nitropyridine and involving intermediates 3-chloro-2-hydroxy-5-nitropyridine, 2,3-dichloro-5-nitropyridine, (5,6-dichloropyridin-3-yl)(2,2-dimethoxyethyl)amine, allyl(5,6-dichloropyridin-3-yl)(2,2-dimethoxyethyl)amine, 2-(S)-hydroxyamino-2-phenylethanol, 2-[(allyl)(5,6-dichloropyridin-3-yl)amino]acetaldehyde, (3aS,6aS)-2-[5-(5,6-dichloropyridin-3-yl)hexahydropyrrolo[3,4-c]isoxazol-1-yl]-2-(S)-phenylethanol, (3aS,6aS)-5-(5,6-dichloropyridin-3-yl)hexahydropyrrolo[3,4-c]isoxazole and [(3S,4S)-4-amino-1-(5,6-dichloropyridin-3-yl)pyrrolidin-3-yl]methanol.

RX(270) OF 404 COMPOSED OF REACTION SEQUENCE RX(18), RX(19)
AND REACTION SEQUENCE RX(4), RX(5), RX(6), RX(8), RX(10), RX(11), RX(12), RX(13), RX(14), RX(19)

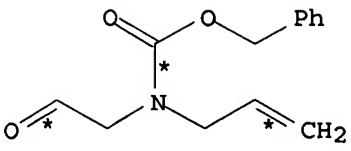
... BB ===> BD...
...K + U + V + 2 AC + AI + BD ===> BH



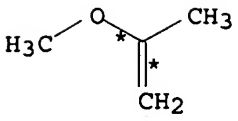
BB BD

START NEXT REACTION SEQUENCE

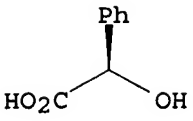
Updated Search



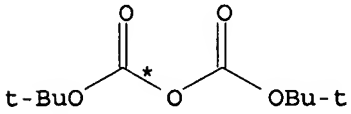
K



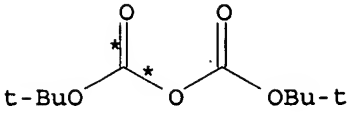
U



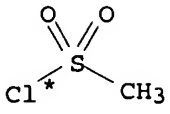
V



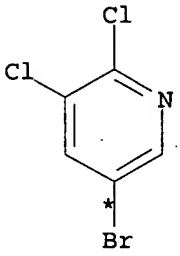
AC



AC

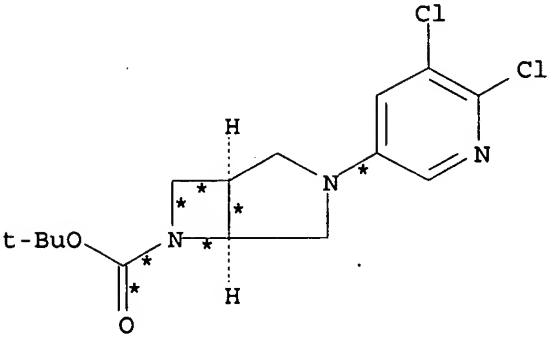


AI



BD

10
STEPS



BH

RX(18) RCT BB 98121-41-6

STAGE(1)
RGT BE 10035-10-6 HBr, BF 7632-00-0 NaNO2
SOL 7732-18-5 Water
CON SUBSTAGE(1) 60 minutes, 0 - 5 deg C
SUBSTAGE(2) 0 - 5 deg C
SUBSTAGE(3) 10 minutes, 0 - 5 deg C

STAGE(2)
RGT BG 7787-70-4 CuBr
SOL 7732-18-5 Water
CON 20 minutes

PRO BD 97966-00-2

RX(4) RCT K 370880-75-4
RGT N 127-09-3 AcONa, O 5470-11-1 H2NOH-HCl
PRO M 370880-76-5
SOL 7732-18-5 Water, 75-05-8 MeCN
CON 20 hours, room temperature

RX(5) RCT M 370880-76-5

Updated Search

```
            STAGE(1)
               SOL  1330-20-7 Xylene
               CON  10 hours, reflux

            STAGE(2)
               RGT  R 64-19-7 AcOH, S 7440-66-6 Zn
               CON  SUBSTAGE(1) reflux -> 15 deg C
                    SUBSTAGE(3) 3 hours, room temperature

         PRO  Q 252770-09-5

RX(6)    RCT  Q 252770-09-5, U 116-11-0

            STAGE(1)
               SOL  67-64-1 Me2CO
               CON  overnight, room temperature

            STAGE(2)
               RCT  V 611-71-2
               SOL  67-64-1 Me2CO
               CON  SUBSTAGE(1) room temperature
                    SUBSTAGE(2) 48 hours, room temperature

         PRO  W 252770-03-9

RX(8)    RCT  W 252770-03-9

            STAGE(1)
               RGT  AE 7664-93-9 H2SO4
               SOL  7732-18-5 Water, 64-17-5 EtOH
               CON  16 hours, room temperature

            STAGE(2)
               RCT  AC 24424-99-5
               RGT  D 1310-73-2 NaOH
               SOL  7732-18-5 Water, 64-17-5 EtOH
               CON  SUBSTAGE(1) room temperature, pH 10
                    SUBSTAGE(2) 10 - 20 deg C
                    SUBSTAGE(3) 4 hours, room temperature

         PRO  AD 246510-69-0
         NTE  stereoselective

RX(10)   RCT  AD 246510-69-0, AI 124-63-0

            STAGE(1)
               RGT  AK 121-44-8 Et3N
               SOL  75-09-2 CH2Cl2
               CON  SUBSTAGE(1) 0.51 hours, -10 deg C
                    SUBSTAGE(2) -10 deg C -> room temperature

            STAGE(2)
               RGT  E 7732-18-5 Water

         PRO  AJ 246510-70-3

RX(11)   RCT  AJ 246510-70-3
         RGT  AN 76-05-1 F3CCO2H
         PRO  AM 799279-83-7
         SOL  75-09-2 CH2Cl2
         CON  1 hour, room temperature


Updated Search
```

RX(12) RCT AM 799279-83-7
RGT D 1310-73-2 NaOH
PRO AO 370881-43-9
SOL 7732-18-5 Water, 64-17-5 EtOH
CON SUBSTAGE(1) room temperature, pH 12
SUBSTAGE(2) 1.5 hours, room temperature -> 60 deg C

RX(13) RCT AO 370881-43-9, AC 24424-99-5
PRO AP 799279-84-8
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 0.3 hours, room temperature
SUBSTAGE(2) 0.5 - 1 hour, room temperature

RX(14) RCT AP 799279-84-8
RGT AR 1333-74-0 H2
PRO AQ 799279-81-5
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH
CON 10 hours, room temperature

RX(19) RCT AQ 799279-81-5, BD 97966-00-2
RGT BI 161265-03-8 Phosphine, 1,1'-(9,9-dimethyl-9H-xanthene-4,5-diyl)bis[1,1-diphenyl-, BJ 865-48-5 NaOBu-t
PRO BH 799279-86-0
CAT 51364-51-3 Ph2-pentadienone Pd
SOL 108-88-3 PhMe
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) 2 hours, room temperature -> 90 deg C

L3 ANSWER 2 OF 9 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 142:134428 CASREACT
TITLE: The syntheses of 3-substituted 4-(pyridin-2-ylthio)indoles via Leimgruber-Batcho indole synthesis
AUTHOR(S): Srisook, Ekaruth; Chi, Dae Yoon
CORPORATE SOURCE: Department of Chemistry, Inha University, Inchon, 402-751, S. Korea
SOURCE: Bulletin of the Korean Chemical Society (2004), 25(6), 895-899
CODEN: BKCSDE; ISSN: 0253-2964
PUBLISHER: Korean Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A new family of radioligands, 3-(amino- and hydroxymethyl)-4-(5-iodopyridin-2-ylthio)indoles, combining characteristically distinct moieties proven to impart successful binding ability in a variety of structurally diverse selective serotonin reuptake inhibitors recently published. Described in this article are the syntheses of 3-substituted 4-(5-iodopyridin-2-ylthio)-indoles, featuring successful adaptation of the modified Leimgruber-Batcho indole synthesis onto the key intermediate 1-(5-iodopyridin-2-ylthio)-2-methyl-3-nitrobenzene prepared from the nucleophilic aromatic substitution of chloropyridine with thiophenol.

RX(2) OF 97 ...H ===> C...

Updated Search

H (2) C
YIELD 41%

RX(2) RCT H 20511-12-0

STAGE(1)
RGT I 7647-01-0 HCl
SOL 7732-18-5 Water
CON 10 minutes, 0 deg C

STAGE(2)
RGT J 7632-00-0 NaNO2, K 7758-89-6 CuCl
CON overnight, room temperature

PRO C 69045-79-0
REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 9 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 141:366121 CASREACT
TITLE: Preparation of dibenzo[b,f]furan-1-carboxamides, 9H-carbazole-4-carboxamides, and dibenzo[b,d]thiophene-4-carboxamides as PDE4 inhibitors for the treatment of inflammatory and allergic disorders
INVENTOR(S): Gopalan, Balasubramanian; Gharat, Laxmikant Atmaram; Lakdawala, Aftab Dawoodbhai; Karaunakaran, Usha
PATENT ASSIGNEE(S): Glenmark Pharmaceuticals Ltd., India
SOURCE: PCT Int. Appl., 121 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004089940	A1	20041021	WO 2004-IB355	20040211
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
IN 2003MU00363	A	20050304	IN 2003-MU363	20030411
AU 2004228453	A1	20041021	AU 2004-228453	20040211
CA 2522023	A1	20041021	CA 2004-2522023	20040211
EP 1620429	A1	20060201	EP 2004-710093	20040211
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,				

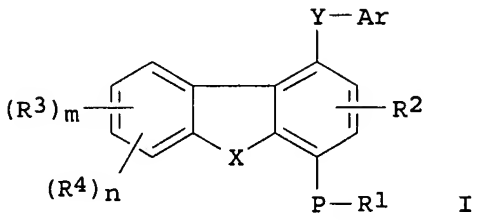
Updated Search

IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

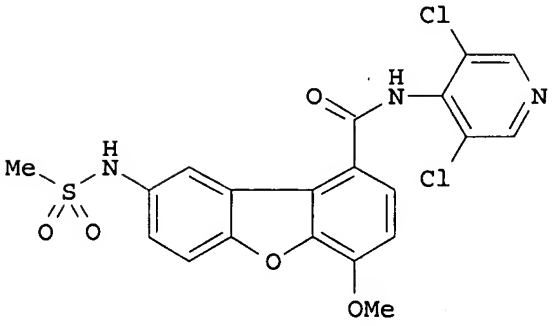
BR 2004009747	A	20060509	BR 2004-9747	20040211
CN 1829711	A	20060906	CN 2004-80016048	20040211
JP 2006522789	T	20061005	JP 2006-506259	20040211
NZ 542882	A	20071026	NZ 2004-542882	20040211
US 2005027129	A1	20050203	US 2004-821642	20040409
US 7223789	B2	20070529		
MX 2005PA10948	A	20060531	MX 2005-PA10948	20051011
ZA 2005008240	A	20060531	ZA 2005-8240	20051012
NO 2005005316	A	20060111	NO 2005-5316	20051110
US 2007105854	A1	20070510	US 2006-536434	20060928
US 2007105855	A1	20070510	US 2006-536448	20060928
PRIORITY APPLN. INFO.:			IN 2003-MU363	20030411
			US 2003-519967P	20031113
			WO 2004-IB355	20040211
			US 2004-821642	20040409

OTHER SOURCE(S): MARPAT 141:366121

GI



I



II

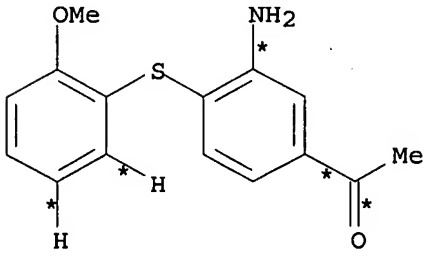
AB Title heterocyclic tricycles I [wherein R1-R3, R5, R6, Ra = independently H, (un)substituted (cyclo)alkyl, (cyclo)alkenyl, alkynyl, (hetero)aryl, heterocyclyl(alkyl), etc.; R4 = NR5R6, heterocyclyl; Ar = (un)substituted aryl(alkyl), heterocyclyl, heteroaryl; X = O, SO0-2, NRa; Y = CONR7, NR7SO0-2, SO0-2NR7, NR7CO; R7 = H, OH, ORa, (un)substituted alkyl, aryl, heterocyclyl; P = O, S; m = 0-3; n = 1-4; and tautomers, regioisomers, stereoisomers, enantiomers, diastereomers, polymorphs, N-oxides, pharmaceutically acceptable salts, solvates, and compns. thereof] were prepared as phosphodiesterase type 4 (PDE4) inhibitors. For example, N-(3,5-dichloropyrid-4-yl)-4-methoxy-8-aminodibenzo[b,f]furan-1-carboxamide (prepared in six steps from isovanillin, 4-fluoronitrobenzene, and 4-amino-3,5-dichloropyridine) was coupled with methanesulfonyl chloride in THF and pyridine to give the sulfonamide II. The latter inhibited the PDE4-induced conversion of [3H] cAMP to the corresponding [3H] 5'-AMP with IC50 of 0.5058 nM. Thus, I and their pharmaceutical compns. are useful for the treatment of immune disorders, inflammatory

Updated Search

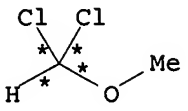
conditions, allergic conditions, CNS diseases, and insulin resistant diabetes (no data).

RX(500) OF 523 COMPOSED OF RX(84), RX(85), RX(86), RX(87), RX(88), RX(89), RX(81)

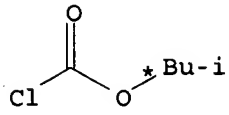
RX(500) FL + FU + CG + X ===> FH



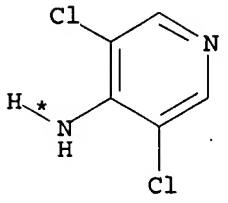
FL



FU

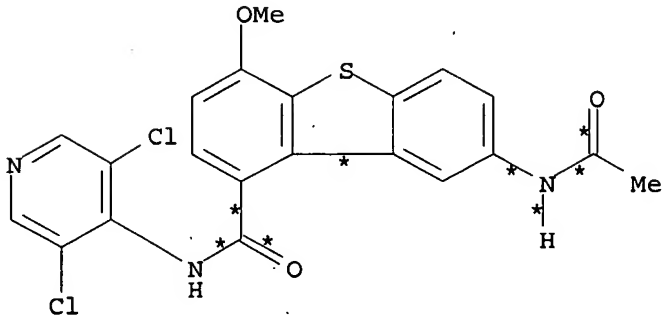


CG



X

7 STEPS



●2 Na

FH

RX(84) RCT FL 19688-56-3

STAGE(1)
RGT EI 7647-01-0 HCl
SOL 7732-18-5 Water

Updated Search

```
              CON   room temperature -> <5 deg C

            STAGE(2)
              RGT   FN 7632-00-0 NaNO2
              CON   SUBSTAGE(1) <5 deg C
                    SUBSTAGE(2) 30 minutes, <5 deg C

            STAGE(3)
              RGT   FO 13755-29-8 Na[BF4]
              CON   SUBSTAGE(1) <5 deg C
                    SUBSTAGE(2) 30 minutes, <5 deg C

            STAGE(4)
              RGT   FP 7664-93-9 H2SO4, FQ 1317-39-1 Cu2O
              SOL   7732-18-5 Water
              CON   SUBSTAGE(2) 15 - 30 minutes

          PRO   FM 778577-00-7

RX(85)    RCT   FM 778577-00-7
          RGT   FS 5470-11-1 H2NOH-HCl, BC 1310-73-2 NaOH
          PRO   FR 778577-01-8
          SOL   67-56-1 MeOH, 7732-18-5 Water
          CON   SUBSTAGE(1) room temperature
                SUBSTAGE(2) 6 - 7 hours, reflux

RX(86)    RCT   FR 778577-01-8

            STAGE(1)
              RGT   Y 7719-09-7 SOCl2
              SOL   109-99-9 THF
              CON   SUBSTAGE(2) 30 minutes

            STAGE(2)
              SOL   7732-18-5 Water

          PRO   FT 778577-02-9

RX(87)    RCT   FU 4885-02-3, FT 778577-02-9

            STAGE(1)
              RGT   FW 7646-78-8 SnCl4
              SOL   75-09-2 CH2Cl2
              CON   SUBSTAGE(1) room temperature -> -10 deg C
                    SUBSTAGE(2) -10 deg C
                    SUBSTAGE(3) 30 minutes, -10 deg C -> room temperature

            STAGE(2)
              SOL   7732-18-5 Water

          PRO   FV 778577-03-0

RX(88)    RCT   FV 778577-03-0
          RGT   FY 7758-19-2 NaOClO, FZ 5329-14-6 Sulfamic acid
          PRO   FX 778577-04-1
          SOL   109-99-9 THF, 7732-18-5 Water
          CON   SUBSTAGE(1) room temperature
                SUBSTAGE(2) 5 minutes, 10 deg C
                SUBSTAGE(3) 30 minutes, 10 deg C

RX(89)    RCT   CG 543-27-1, FX 778577-04-1


Updated Search
```

STAGE(1)
RGT DY 7087-68-5 EtN(Pr-i)2
SOL 68-12-2 DMF
CON SUBSTAGE(1) room temperature -> -20 deg C
SUBSTAGE(2) -20 deg C
SUBSTAGE(3) 10 - 12 hours

STAGE(2)
SOL 7732-18-5 Water

PRO FG 778577-05-2

RX(81) RCT X 22889-78-7, FG 778577-05-2

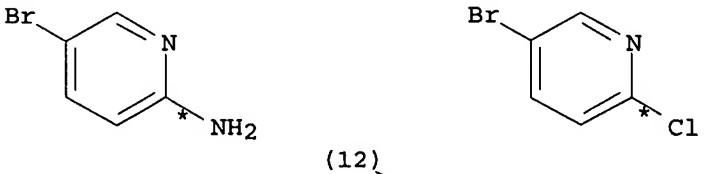
STAGE(1)
RGT Z 7646-69-7 NaH
SOL 68-12-2 DMF
CON SUBSTAGE(2) 30 minutes

STAGE(2)
SOL 7732-18-5 Water

PRO FH 778576-99-1
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 4 OF 9 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 141:140291 CASREACT
TITLE: An efficient route to 6-(het)aryl-2-methyl-2,3-dihydro-1H-pyridin-4-ones as potential nAChRs ligands
AUTHOR(S): Leflemme, Nicolas; Dallemagne, Patrick; Rault, Sylvain
CORPORATE SOURCE: Centre d'Etudes et de Recherche sur le Medicament de Normandie, UFR des Sciences Pharmaceutiques, Caen, 14032, Fr.
SOURCE: Tetrahedron (2004), 60(22), 4861-4865
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A new efficient pathway to synthesize 6-(het)aryl-2-methyl-2,3-dihydro-1H-pyridin-4-ones is described. This reaction sequence involved, as a key step, a Suzuki cross-coupling reaction between various boronic acids and an 6-iodo-2,3-dihydropyridin-4-one. A final deprotecting step furnished the attempted products.

RX(12) OF 46 AF ===> K...



AF

K
YIELD 56%

Updated Search

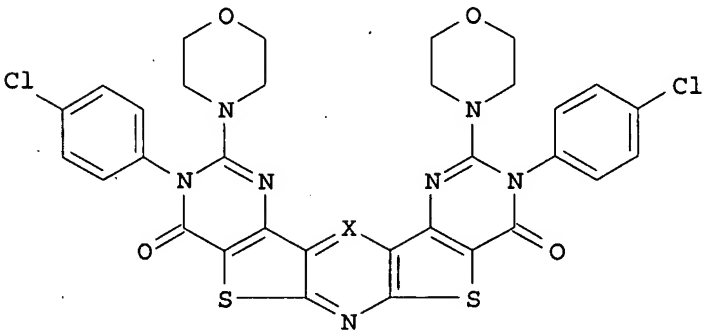
RX(12) RCT AF 1072-97-5

STAGE(1)
RGT AG 7632-00-0 NaNO2, E 7647-01-0 HCl
CON 0 deg C

STAGE(2)
RGT AH 7758-89-6 CuCl
CON 0 deg C -> room temperature

PRO K 53939-30-3
REFERENCE COUNT: 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 5 OF 9 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 140:163819 CASREACT
TITLE: Synthesis of pyrido and pyrazinodithienodipyrimidine-4,8(3H,9H)-dione derivatives by the aza-Wittig methodology
AUTHOR(S): Vilarelle, David Vazquez; Veira, Carlos Peinador; Quintela Lopez, Jose M.
CORPORATE SOURCE: Facultad de Ciencias, Departamento de Quimica Fundamental, Universidad de La Coruna, La Coruna, E-15071, Spain
SOURCE: Tetrahedron (2004), 60(2), 275-283
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

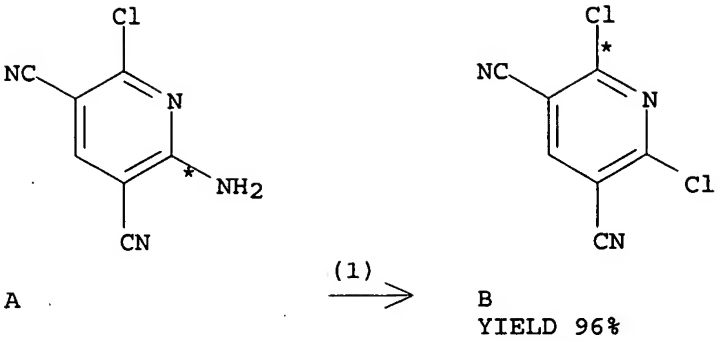


I

AB A one-pot synthesis of the hitherto unreported pyrido[5'',6'':4,5;3''2'':4',5']dithieno[3,2-d:3',2'-d']dipyrimidine-4,8(3H,9H)-diones, e.g. I (X = CH), and pyrazino[5'',6'':4,5;3''2'':4',5']dithieno[3,2-d:3',2'-d']dipyrimidine-4,8(3H,9H)-diones, e.g. I (X = N) pentaheterocyclic systems, based on the tandem aza-Wittig heterocumulene-mediated annulation strategy, is described.

RX(1) OF 157 A ===> B...

Updated Search



A → B

YIELD 96%

RX(1) RCT A 51768-01-5

STAGE(1)
RGT C 7447-39-4 CuCl2, D 110-46-3 Isoamyl nitrite
SOL 75-05-8 MeCN
CON 5 hours, 65 deg C

STAGE(2)
RGT E 7647-01-0 HCl
SOL 7732-18-5 Water
CON room temperature, acidify

PRO B 151229-84-4

REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 6 OF 9 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 140:93833 CASREACT

TITLE: An Efficient Two-Step Total Synthesis of the Quaterpyridine Nemertelline

AUTHOR(S): Bouillon, Alexandre; Voisin, Anne Sophie; Robic, Audrey; Lancelot, Jean-Charles; Collot, Valerie; Rault, Sylvain

CORPORATE SOURCE: UFR des Sciences Pharmaceutiques, Centre dEtudes et de Recherche sur le Medicament de Normandie, Caen, 14032, Fr.

SOURCE: Journal of Organic Chemistry (2003), 68(26), 10178-10180
CODEN: JOCEAH; ISSN: 0022-3263

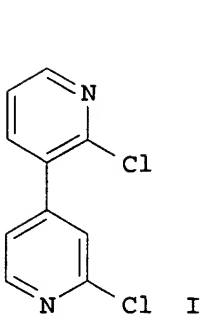
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

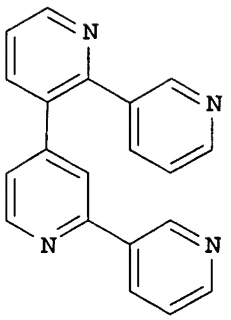
LANGUAGE: English

GI

Updated Search



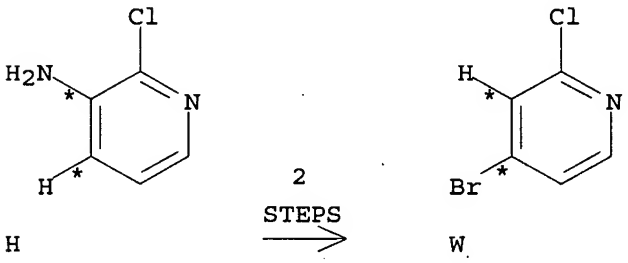
I



II

AB Regioselective and univocal Suzuki cross-coupling reactions performed on halopyridinyl boronic acids provide a flexible and versatile route to a multigram scale synthesis of 2,2'-dichloro-3,4'-bipyridine (I), which allows couplings with excess pyridin-3-yl boronic acid to give a new and efficient two-step rapid synthesis of nemertelline (II), the quaterpyridine neurotoxin isolated from a Hoplonemertine sea worm.

RX(13) OF 44 COMPOSED OF RX(4), RX(6)
RX(13) H ===> W



H W

RX(4) RCT H 6298-19-7
RGT O 10035-10-6 HBr, K 7632-00-0 NaNO2, P 7787-70-4 CuBr
PRO N 52200-48-3
SOL 7732-18-5 Water

RX(6) RCT N 52200-48-3

STAGE(1)
RGT X 4111-54-0 LiN(Pr-i)2
CAT 7726-95-6 Br2
CON -78 - -50 deg C

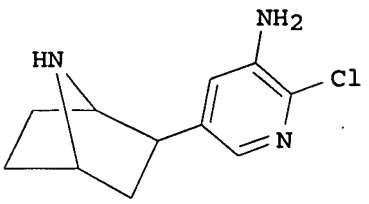
STAGE(2)
RGT J 7647-01-0 HCl
SOL 7732-18-5 Water

PRO W 73583-37-6
NTE regioselective

REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Updated Search

L3 ANSWER 7 OF 9 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 137:353202 CASREACT
TITLE: Synthesis, Nicotinic Acetylcholine Receptor Binding, and Antinociceptive Properties of 2-exo-2-(2',3'-Disubstituted 5'-pyridinyl)-7-azabicyclo[2.2.1]heptanes: Epibatidine Analogues
AUTHOR(S): Carroll, F. Ivy; Lee, Jeffrey R.; Navarro, Hernan A.; Ma, Wei; Brieaddy, Lawrence E.; Abraham, Philip; Damaj, M. I.; Martin, Billy R.
CORPORATE SOURCE: Chemistry and Life Sciences, Research Triangle Institute, Research Triangle Park, NC, 27709, USA
SOURCE: Journal of Medicinal Chemistry (2002), 45(21), 4755-4761
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

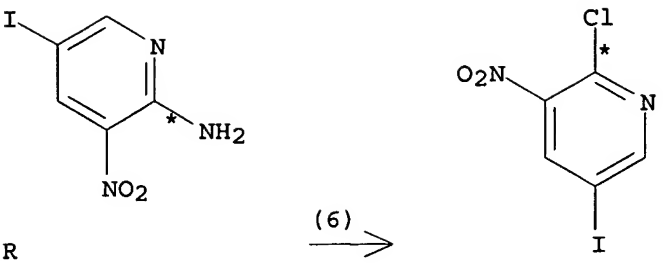


I

AB A number of 2',3'-disubstituted epibatidine analogs were synthesized and evaluated in vitro for potency at nicotinic acetylcholine receptors (nAChRs) and in vivo for antinociception activity in the tail-flick and hot-plate models of acute pain and for their ability to affect core body temperature Compds. that possessed electron-withdrawing groups (F, Cl, Br, and I) in both the 2'- and the 3'-positions showed affinities at the nAChR similar to epibatidine. However, in vivo efficacy did not correlate with affinity. 2-Exo-(3'-Amino-2'-chloro-5'-pyridinyl)-7-azabicyclo[2.2.1]heptane (I), an epibatidine analog possessing an electron-releasing amino group in the 3'-position, produced the highest affinity. Compound I was also the most selective epibatidine analog with a Ki of 0.001 nM at αβ nAChRs, which is 26 times greater than that of epibatidine, and a αβ/α7 Ki ratio of 14 000, twice that of epibatidine. In vivo testing revealed that this compound potently inhibited nicotine-induced antinociception with AD50 values below 1 μg/kg. Surprisingly, this same compound was also an agonist at higher doses (ED50 .apprx.20 μg/kg). Thus, the addition of the 3'-amino group to epibatidine confers potent antagonist activity to the compound with little effect on agonist activity. 2,3-Disubstituted epibatidine analogs possessing a 2'-amino group combined with a 3'-bromo or 3'-iodo group showed in vitro and in vivo nAChR properties similar to nicotine.

RX(6) OF 95 ...R ===> W...

Updated Search



R

W
YIELD 36%

RX(6) RCT R 25391-57-5

STAGE(1)
RGT X 7647-01-0 HCl
SOL 7732-18-5 Water

STAGE(2)
RGT D 7632-00-0 NaNO2, Y 7758-89-6 CuCl

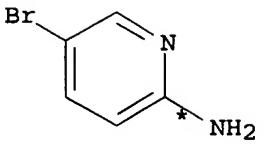
STAGE(3)
RGT E 1336-21-6 NH4OH
SOL 7732-18-5 Water

PRO W 426463-05-0
REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 8 OF 9 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 137:125209 CASREACT
TITLE: Synthesis of novel halopyridinylboronic acids and esters. Part 1: 6-Halopyridin-3-yl-boronic acids and esters
AUTHOR(S): Bouillon, Alexandre; Lancelot, Jean-Charles; Collot, Valerie; Bovy, Philippe R.; Rault, Sylvain
CORPORATE SOURCE: Centre d'Etudes et de Recherche sur le Medicament de Normandie, UFR des Sciences Pharmaceutiques, Universite de Caen, Caen, 14032, Fr.
SOURCE: Tetrahedron (2002), 58(14), 2885-2890
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB This paper describes a general method for the synthesis and isolation of novel 6-halo-pyridin-3-yl-boronic acids and esters. These compds. are prepared taking in account a regioselective halogen-metal exchange with a trialkyl borate starting from 2,5-dihalopyridines. All substrates studied to date provided a single regioisomeric boronic acid or ester product. Addnl., these compds. have been found to undergo Pd-catalyzed coupling with a range of aryl halides and authorize a strategy to produce new pyridines libraries. Thus, lithiation of 2,5-dibromopyridine with BuLi in Et2O followed by borylation with B(OiPr)3 and sequential basic hydrolysis gave 75% 2-bromo-5-pyridylboronic acid.

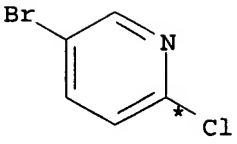
RX(4) OF 24 M ===> I...

Updated Search



M

(4)

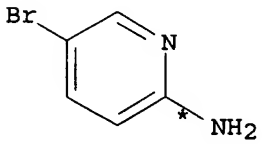


I
YIELD 55%

RX(4) RCT M 1072-97-5
RGT F 7647-01-0 HCl, N 7632-00-0 NaNO2, O 7758-89-6 CuCl
PRO I 53939-30-3
SOL 7732-18-5 Water
REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

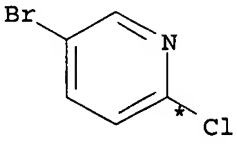
L3 ANSWER 9 OF 9 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 135:107263 CASREACT
TITLE: Synthesis of multifunctional ligands: a 2,9-diaryl-1,10-phenanthroline/2,2':6',2''-terpyridine conjugate
AUTHOR(S): Belfrekh, N.; Dietrich-Buchecker, C.; Sauvage, J.-P.
CORPORATE SOURCE: Laboratoire de Chimie Organo-Minerale, Faculte de Chimie, rue Blaise Pascal, 4, UMR 7513 du CNRS, Universite Louis Pasteur, Strasbourg, 67070, Fr.
SOURCE: Tetrahedron Letters (2001), 42(15), 2779-2781
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The synthesis of a ligand including a 1,10-phenanthroline and a 2,2':6',2''-terpyridine separated by a 1,3-phenylene spacer is presented. The different aromatic C-C bonds were generated by reactions with organolithium compds., and by Stille and Suzuki couplings.

RX(1) OF 44 A ===> B...



A

(1)



B
YIELD 40%

RX(1) RCT A 1072-97-5

STAGE(1)
RGT C 7647-01-0 HCl, D 7632-00-0 NaNO2
SOL 7732-18-5 Water

STAGE(2)

Updated Search

RGT E 7758-89-6 CuCl

PRO B 53939-30-3
NTE literature prepn.
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=>

Updated Search

L3 ANSWER 8 OF 9 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 137:125209 CASREACT
TITLE: Synthesis of novel halopyridinylboronic acids and esters. Part 1: 6-Halopyridin-3-yl-boronic acids and esters
AUTHOR(S): Bouillon, Alexandre; Lancelot, Jean-Charles; Collot, Valerie; Bovy, Philippe R.; Rault, Sylvain
CORPORATE SOURCE: Centre d'Etudes et de Recherche sur le Medicament de Normandie, UFR des Sciences Pharmaceutiques, Universite de Caen, Caen, 14032, Fr.
SOURCE: Tetrahedron (2002), 58(14), 2885-2890
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB This paper describes a general method for the synthesis and isolation of novel 6-halo-pyridin-3-yl-boronic acids and esters. These compds. are prepared taking in account a regioselective halogen-metal exchange with a trialkyl borate starting from 2,5-dihalopyridines. All substrates studied to date provided a single regioisomeric boronic acid or ester product. Addnl., these compds. have been found to undergo Pd-catalyzed coupling with a range of aryl halides and authorize a strategy to produce new pyridines libraries. Thus, lithiation of 2,5-dibromopyridine with BuLi in Et20 followed by borylation with B(OiPr)3 and sequential basic hydrolysis gave 75% 2-bromo-5-pyridylboronic acid.

RX(4) OF 24 M ===> I...

M → I
YIELD 55%

RX(4) RCT M 1072-97-5
RGT F 7647-01-0 HCl, N 7632-00-0 NaNO2, O 7758-89-6 CuCl
PRO I 53939-30-3
SOL 7732-18-5 Water
REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Updated Search

L3 ANSWER 9 OF 9 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 135:107263 CASREACT
TITLE: Synthesis of multifunctional ligands: a 2,9-diaryl-1,10-phenanthroline/2,2':6',2''-terpyridine conjugate
AUTHOR(S): Belfrekh, N.; Dietrich-Buchecker, C.; Sauvage, J.-P.
CORPORATE SOURCE: Laboratoire de Chimie Organo-Minerale, Faculte de Chimie, rue Blaise Pascal, 4, UMR 7513 du CNRS, Universite Louis Pasteur, Strasbourg, 67070, Fr.
SOURCE: Tetrahedron Letters (2001), 42(15), 2779-2781
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The synthesis of a ligand including a 1,10-phenanthroline and a 2,2':6',2''-terpyridine separated by a 1,3-phenylene spacer is presented. The different aromatic C-C bonds were generated by reactions with organolithium compds., and by Stille and Suzuki couplings.

RX(1) OF 44 A ===> B...

A

B
YIELD 40%

RX(1) RCT A 1072-97-5

STAGE(1)
RGT C 7647-01-0 HCl, D 7632-00-0 NaNO2
SOL 7732-18-5 Water

STAGE(2)
RGT E 7758-89-6 CuCl

PRO B 53939-30-3
NTE literature prepn.
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=>

Updated Search